INTRODUCTION TO COMPUTER TOOL CAFE

On initiative of the pilot study directors and the Danish host, participants involved with development or working with PC-tools and databases supporting cleaner production were invited to present and demonstrate these tools. The computer tool cafe was organized as a hands-on demonstration event. Descriptions of the demonstrated tools are presented here.

Computer Tool Cafe

CHEMICAL LIFE CYCLE DATABASE.
Demonstrated by
Michael Overcash, USA

Description:
Extract from the abstract to Concepción, J-G., Seungdo, K. and Overcash, M.R. (2000): Methodology for Developing Gate-to-Gate Life Cycle Inventory Information. Int. J. LCA, 5 (2000)
This work presents an option to generate gata-to-gate life cycle information of chemical substances, based on a transparent methodology of chemical engineering process design (an ab initio approach). In the broader concept of a life cycle inventory (LCI), the information of each gate-to-gate module can be linked accordingly in a production chain, including the extraction of raw materials, transportation, disposal, reuse, etc. to provide a full cradle to gate evaluation. The methodology aims to help the LCA practitioner to obtain a fair and transparent estimate of LCI data when the information is not readily available from industry or literature. The LCI

information from this methodology can be used more directly in exploring engineering and chemistry changes to improve manufacturing processes.

Further information: Overcash, M. Chemical Life Cycle Inventory Library, North Carolina State University, Raleigh, N.C. 27695-7905, 2000. E-mail: overcash@eos.ncsu.edu

CAPEC SOFTWARE TOOLS FOR CHEMICAL AND PROCESS SYSTEM ENGINEERING.
Demonstrated by
Peter Harper, Denmark

Description

ProCamd: Program based on computer aided molecular design that can be used for solvent selection, search and design

ProPred: Pure component property prediction package. An easy to use program package that is able to predict pure component properties of most organic compounds from molecular structural information.

ICAS: An integrated computer aided system through which various problems related to a process, product and/or operation could be investigated and solved efficiently, consistently and reliably. Various computer aided tools such as proCamd, proPred, and design tool-box have been integrated with databases and simulation engines within ICAS.

CAPEC database: A database of pure component and mixture properties and, solvent properties for a very large range of compounds, including amino acids and steroids.

Further information: Rafique Gani, Deparment of Chemical Engineering, Technical University of Denmark, e-mail: rag@popeye.kt.dtu.dk or www.capec.kt.dt.dk

Explaining the EDIP LCA-software needs standing argumentation

THE EDIP (ENVIRONMENTAL DESIGN OF INDUSTRIAL PRODUCTS) LIFE CYCLE ASSESSMENT TOOL.
Demontrated by
Morten Als Pedersen, Denmark

Description
The EDIP-PC tool, betaversion 2.11 was released by the Danish Environmental Protection Agency in June 1998. The betaversion contains the necessary functionality to support the work process of life cycle based environmental assessment of products and systems. The betaversion 2.11 system contains three functions:
- the Unit Process Database,
- the Modelling Tool and
- the Calculation Facilities.

The EDIP PC-tool contains the neessary functionality to fully support the work process in life cycle based environmental assessment. The in-built Unit Process Database contains approx. 750 process cards, covering all types of systems. Approx. 200 of these are in the category "substances" leaving over 500 unit processes, which are categorized in: materials, auxillary materials, transport systems, production processes, disposal systems/scenarios, energy systems, etc. Unit processes are the basic building blocks of the EDIP Life Cycle Model. The quantitative part of the process data is scalable, making it possible for students and other users to apply the data in other contexts.
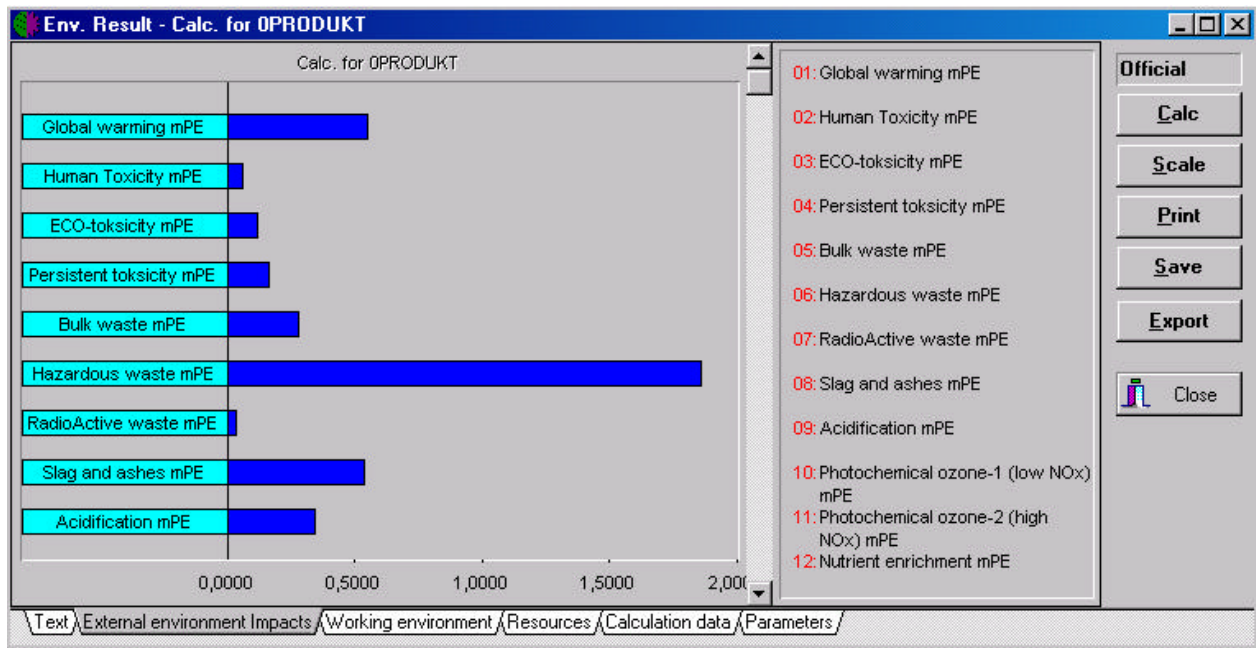
Figure: screen dump from the EDIP tool showing grachical desplay of results

The modelling process is done in a Windows file-manager-alike structure. With the calculation facilities it is possible to calculate an inventory or to assess the environmental impacts for the whole system or any part of this. Above figure shows a graphical display of results.

Further information: Morten Als Pedersen, Department of Manufacturing Engineering and Institute for Product Development, map@ipl.dtu.dk.
Danish version of software and software licence can be obtained at Danish Environmenal Protection Agency Center for Information http://www.mem.dk/butik/ Information on English version can be obtained at Department of Manufacturing Engineering and Institute for Product Development, cm@ipl.dtu.dk

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PARIS II – AN ENVIRONMENTAL FRIENDLY CHEMICAL SUBSTITUTION IN INDUSTRY.
Demontrated by
Dan Murray, USA

Description
PARIS II is a solvent design software. It has been completed and transferred to the private enterprise TDS, Inc. (New York City) for marketing. Beta testing has just started with 50 companies participating. PARIS II program designs, in the computer, solvent mixtures with reduced environmental impact (such as toxicity and other measures) that match the property profile of the solvent mixture being used currently.

User inputs are chemical composition of solvent, operating conditions, and the tolerance ranges for solvent physical parameters including environmental parameters and the output of the software analysis is a ranked list of solvents based on closeness in meeting the specified criteria

PARIS II can be used by the designer or producer of solvents or by the solvent user or decision-maker to evaluate the effectiveness and environmental impacts of solvent substitutes or to develop custom solvents to meet specific needs based on chemical properties and environmental considerations.

Further information:
Point of contact at USEPA is e-mail: cabezas.heriberto@epamail.epa.gov.
PARIS II is further described in the paper dated September 16, 1999 entitled Environmental Improvement Toolbox, published by EPA, National Risk Management Research Laboratory, Sustainable Technology Division, Systems Analysis Branch. The toolbox contains a description of fifteen pollution prevention/environmental analysis tools, and is continually updated as tools are refined and new tools added. Point of contact at EPA is e-mail: hoagland.theresa@epamal.epa.gov.
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